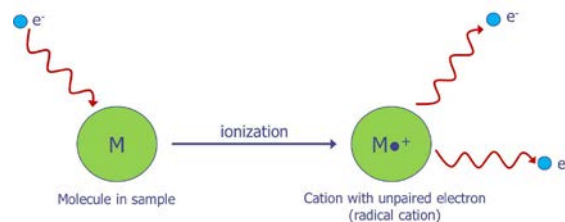


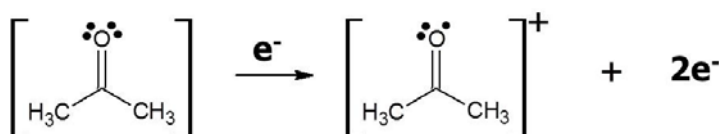
TAD03 – (A4 Notes) Mass Spectrometry

Name

1. A.4.1 Determine the molecular mass of a compound from the molecular ion peak. (3)
- a. Explain ionization:



- b. Using Propanone as an example, explain the mass to charge (m/e) ratio of compounds:



- c. What happens during the ionization of a compound, use propanone as an example again:

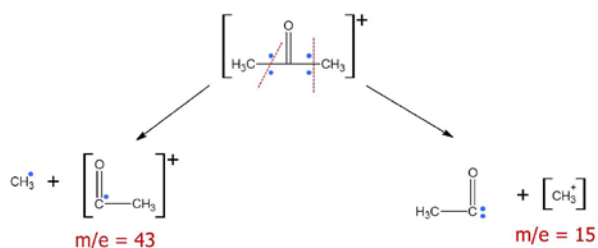
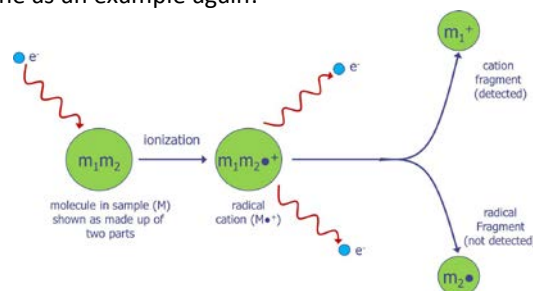
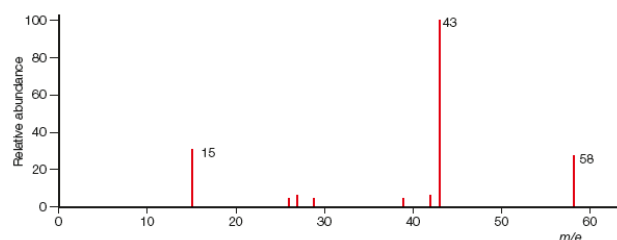


Figure 21.50 Mass spectrum of propanone

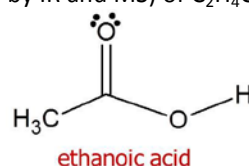
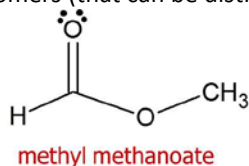


2. A.4.2 Analyze fragmentation patterns in a mass spectrum to find the structure of a compound. (3) Examples of fragments should include: $(M_r - 15)^+$ loss of CH_3 , $(M_r - 17)^+$ loss of OH , $(M_r - 29)^+$ loss of C_2H_5 or CHO , $(M_r - 31)^+$ loss of CH_3O , $(M_r - 45)^+$ loss of COOH

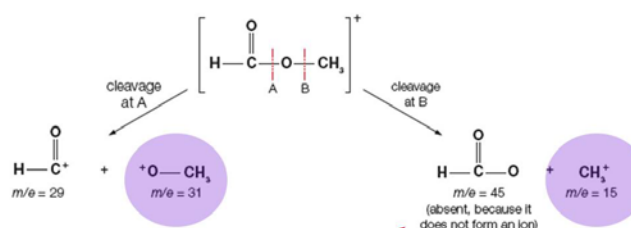
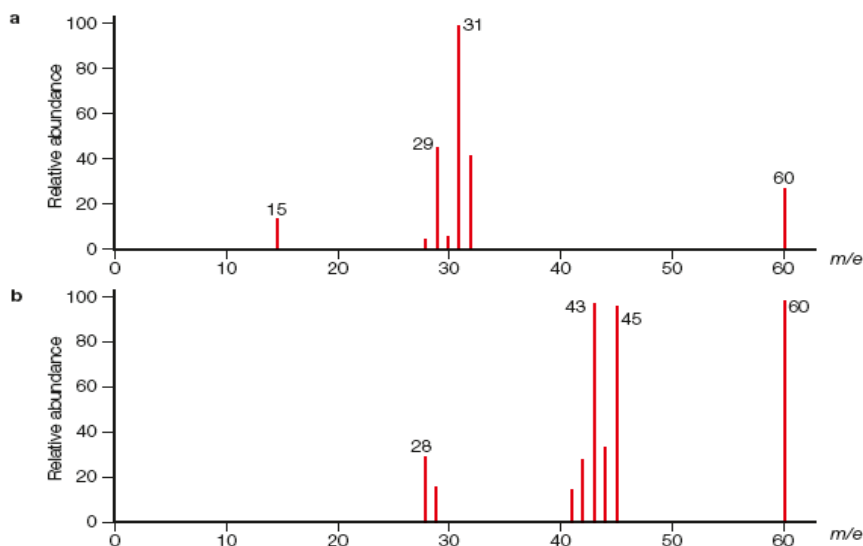
- a. Common Molecular Fragments:

Fragment	m/e	Structural Formula
CH_3^+	15	
OH^+	17	
CH_3CH_2^+ or CHO^+	29	
CH_2NH_2^+	30	
CH_2OH^+ or CH_3O^+	31	
CH_3O^+ or C_3H_7^+	43	
CONH_2^+	44	
COOH^+	45	
C_6H_5^+	77	
$\text{C}_6\text{H}_5\text{CH}_2^+$	91	
$\text{C}_6\text{H}_5\text{CO}^+$	105	

- b. There are two stable isomers (that can be distinguished by IR and MS) of $C_2H_4O_2$

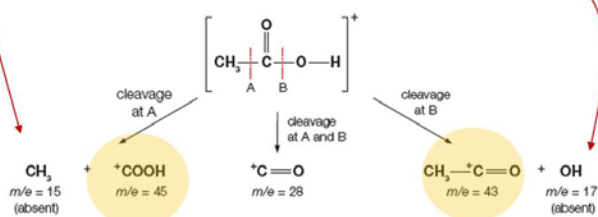


- i. Two things happen to each compound when ionized.
1. The whole compound forms a cation, which peaks are these responsible for?
 2. Each of the cations can be further separated as bonds are cleaved to form reasonably stable (considering the conditions) cations for detection.



IB does not expect you to know where and to what degree compounds will cleave and be stable, but you should be able to problem solve a similar problem

no charge = no peak



- c. Compounds with various isotopes:

- i. Explain why chloroethane, CH_3CH_2Cl , MS data contains 'pairs' of peaks

